

Magnetic impurities in the two-band s_{\pm} -wave superconductors

JIAN LI AND YUPENG WANG

Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

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Abstract. - We investigate the effects of magnetic impurities in a superconducting state with s_{\pm} pairing symmetry. Within a two-band model, we find that the intra-band magnetic scattering serves as a pair breaker while the inter-band magnetic scattering preserves pairing and hardly affects transition temperature in the Born limit. We also show that the same physics can persist beyond the weak scattering region. Our results coincide with recent experimental measurements in iron-based superconductors and thus provides an indirect evidence of the possible s_{\pm} pairing symmetry in these materials.

The iron-based superconductors have attracted much attention since the compound $LaFeAsO_{1-x}F_x$ was found superconducting with $T_c = 26K$ [1]. Accompanied with the increasing transition temperature over 40K [2] and finally up to 55K [3], these new superconductors are considered as the second family of high-temperature superconductors after the cuprates. Though much efforts have been made and great progress has been achieved experimentally, the superconducting mechanism and the pairing symmetry are still unclear because of the complexity of multi-orbital nature and possible strong electron-electron correlation in these materials. The angle-resolved photoemission spectroscopy (ARPES) [4], the Andreev reflection [5] and the penetration depth [6] experiments directly showed fully gaped superconductivity while the nuclear-magnetic-resonance (NMR) indicates a strong deviation from that of single band s -wave superconductors [7]. Simultaneously, the s_{\pm} pairing symmetry was proposed and widely discussed by many authors theoretically [8]. With this kind of pairing symmetry, fully opened gap located in the hole pocket around the Γ point and electron pocket around the M point have opposite signs. The s_{\pm} pairing symmetry is consistent with the ARPES results and also coincides with the NMR results providing the presence of strong impurities [9] and thus becomes a very promising candidate to account for the main physics of the iron-based superconductors.

To distinguish the pairing symmetry experimentally, we note that the effects of impurities in superconducting states can be very different for different pairing symme-

tries. Very recently, superconductivity in both 1111 and 122 systems has been induced by doping magnetic elements Co [10,11]. These experiments share some common features. First, the superconductivity in these materials shows high tolerance with the disorder induced by the Co -doping. Second, the suppression of the transition temperature is not so significant but still much stronger than the F -doped materials. The second point can be easily understood because the F -doping happens in the LaO layers while the Co -doping happens in the $FeAs$ layers which are crucial to the superconductivity. However, a later experiment [12] on Zn -doped $LaFeAsO$ shows that the superconductivity is almost unperturbed by the Zn -doping, though it happened in the $FeAs$ layers. This strongly indicates that the non-magnetic impurities are unlikely to affect the superconductivity, in accordance with s -wave pairing symmetry. Meanwhile, magnetic impurities can depress the transition temperature but not so significant as in the conventional s -wave superconductors. A. E. Karkin et al used fast neutron irradiation to induce disorder in $LaFeAsO_{0.9}F_{0.1}$ and found the depression of transition temperature can be qualitatively described by Abrikosov-Gorkov (AG) theory with magnetic impurities [13]. However, such depression is also much slower than that predicted by the AG theory (see Fig.10 in [13]).

To solve this puzzle, we propose a model in this letter to describe the behavior of the magnetic impurities in an s_{\pm} -wave superconductor and show how the inter-band magnetic impurity scattering processes may preserve the pairs and effectively weaken the reduction of transition

temperature. Our theoretical results give a reasonable explanation of the experimental data.

We start with a model consisting of two perfect nested bands, i.e., an electron Fermi pocket and a hole Fermi pocket. The details of the band structure is neglected and the superconducting order parameters located in each band have same magnitude but reversed signs as in Refs. [14, 15]. For convenience, we introduce the Nambu vector

$$\psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, d_{\mathbf{k}\uparrow}, d_{\mathbf{k}\downarrow}, c_{-\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow}^\dagger, d_{-\mathbf{k}\uparrow}^\dagger, d_{-\mathbf{k}\downarrow}^\dagger),$$

here $c_{\mathbf{k}\sigma}$ and $d_{\mathbf{k}\sigma}$ are the annihilation operators in the electron band and the hole band and the band energy $\epsilon_{c,\mathbf{k}} = -\epsilon_{d,\mathbf{k}} = \epsilon_{\mathbf{k}}$, respectively. Here we treat the magnetic impurities as localized spins in the classical limit and the quantum (Kondo) effect of impurities is not under our consideration. In this limit, the magnetic impurity is equivalent to the local magnetic field. Then the interaction matrix due to magnetic impurity scattering is assumed to be

$$V = \frac{1}{2} \begin{pmatrix} J_1 \sigma \cdot \mathbf{S} & J_2 \sigma \cdot \mathbf{S} & 0 & 0 \\ J_2 \sigma \cdot \mathbf{S} & J_1 \sigma \cdot \mathbf{S} & 0 & 0 \\ 0 & 0 & J_1 \sigma_2 \sigma \cdot \mathbf{S} \sigma_2 & J_2 \sigma_2 \sigma \cdot \mathbf{S} \sigma_2 \\ 0 & 0 & J_2 \sigma_2 \sigma \cdot \mathbf{S} \sigma_2 & J_1 \sigma_2 \sigma \cdot \mathbf{S} \sigma_2 \end{pmatrix}$$

Here σ and \mathbf{S} denotes the spin operator of the electrons and magnetic impurities, respectively. Both the intra-band (J_1) and the inter-band (J_2) exchange coupling constants are positive and isotropic in our consideration.

Following the AG theory [16], the renormalized two-band BCS Green's function with randomly distributed impurities of finite concentration n_{imp} reads:

$$G^{-1}(\mathbf{k}, \omega) = G_0^{-1}(\mathbf{k}, \omega) - \sum(\omega) \\ = \begin{pmatrix} i\tilde{\omega} - \epsilon_{\mathbf{k}} & x & -i\tilde{\Delta}\sigma_2 & 0 \\ x & i\tilde{\omega} + \epsilon_{\mathbf{k}} & 0 & i\tilde{\Delta}\sigma_2 \\ i\tilde{\Delta}\sigma_2 & 0 & i\tilde{\omega} + \epsilon_{\mathbf{k}} & x \\ 0 & -i\tilde{\Delta}\sigma_2 & x & i\tilde{\omega} - \epsilon_{\mathbf{k}} \end{pmatrix}, \quad (1)$$

where $G_0(\mathbf{k}, \omega)$ is the Green's function without the impurity; $\sum(\omega)$ is the self energy; $\tilde{\omega}$ and $\tilde{\Delta}$ is the renormalized frequency and superconducting order parameter, respectively. The parameter x is the inter-band scattering induced contribution to the self-energy which can be determined self-consistently. In the Born approximation the self-energy can be written as [17]

$$\sum(\omega) = n_{imp} \int \frac{d^2 k'}{(2\pi)^2} \langle V G(k', \omega) V \rangle_I$$

where $\langle \dots \rangle_I$ means averaging the impurity position. Now the renormalized Green's function can be given self-

consistently with

$$\tilde{\omega} = \omega + \left(\frac{ix}{2\tau_3} + \frac{\tilde{\omega}}{2\tau_1} \right) \frac{1}{\sqrt{\tilde{\Delta}^2 + \tilde{\omega}^2 + x^2}}, \quad (2)$$

$$\tilde{\Delta} = \Delta - \frac{1}{2\tau_2} \frac{\tilde{\Delta}}{\sqrt{\tilde{\Delta}^2 + \tilde{\omega}^2 + x^2}}, \quad (3)$$

$$x = \left(\frac{i\tilde{\omega}}{2\tau_3} - \frac{x}{2\tau_1} \right) \frac{1}{\sqrt{\tilde{\Delta}^2 + \tilde{\omega}^2 + x^2}}, \quad (4)$$

and the spin-flip scattering times:

$$\frac{1}{\tau_1} = \frac{(J_1^2 + J_2^2)}{2} \pi N_F n_{imp} S(S+1),$$

$$\frac{1}{\tau_2} = \frac{(J_1^2 - J_2^2)}{2} \pi N_F n_{imp} S(S+1),$$

$$\frac{1}{\tau_3} = J_1 J_2 \pi N_F n_{imp} S(S+1),$$

with N_F the density of states at the Fermi surface.

With the above equations we obtain

$$\frac{\omega}{\Delta} = u \left[1 - \frac{1}{\tau_S \Delta} \frac{1}{\sqrt{1 + u^2 - (\frac{I}{\Delta})^2}} \right],$$

with $u = \frac{\tilde{\omega}}{\Delta}$ and $I = ix$. The effective pair-breaking parameter is $\alpha \equiv \frac{1}{\tau_S \Delta} = \left(\frac{I}{\tilde{\omega}} \frac{1}{2\tau_3} + \frac{1}{2\tau_1} + \frac{1}{2\tau_2} \right) \frac{1}{\Delta}$.

Now it is clear that the Green's function contains two terms: one is the conventional term as in the single-band s -wave superconductors with the renormalized frequency and superconducting order parameter and the other one is the contribution induced by the inter-band magnetic impurity scattering processes. If the inter-band scattering term x in the renormalized Green's function is neglected, the effective pair-breaking parameter reads $\alpha = \alpha_0 = \left(\frac{1}{2\tau_1} + \frac{1}{2\tau_2} \right) \frac{1}{\Delta} \propto J_1^2$, quite similar to that in the conventional AG theory. However, a non-zero J_2 will change the situation significantly as we shall show below.

Making $i\omega \rightarrow \omega$, the density of states (DOS) is given by:

$$N(\omega) = -\frac{1}{\pi} \text{Im} \int \frac{d^2 k}{(2\pi)^2} G_{11}^R(k, \omega) \\ = N_F \text{Im} \left(\frac{\tilde{\omega}}{\sqrt{\tilde{\Delta}^2 - \tilde{\omega}^2 + x^2}} \right).$$

Numerical results of the DOS for given α_0 and $\lambda = J_2/J_1$ are shown in Fig.1. The densities of states for both the conventional two-band s -wave case and the s_{\pm} -wave case are calculated. The numerical results clearly show that in the conventional s -wave case (left part of Fig.1), the inter-band scattering also depresses the superconducting gap. However, accompanied with the increasing of J_2 , the superconducting gap is growing larger in s_{\pm} -wave case. This strongly indicates that J_1 and J_2 have opposite effects on the gap of s_{\pm} -wave superconductors. It seems that the inter-band magnetic impurity scattering played as a pair

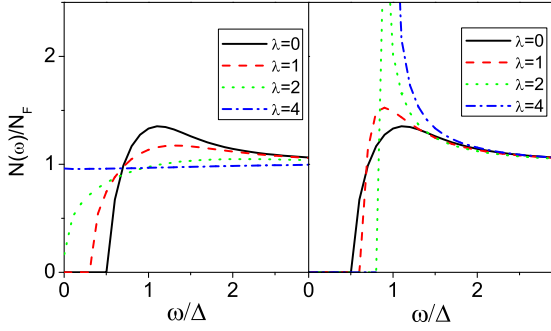


Fig. 1: (Color online) The density of states for $\alpha_0 = 0.2$ and $\lambda = J_2/J_1$. The left part is for the s -wave pairing symmetry and the right one is for s_{\pm} -wave pairing symmetry.

repairee in our system. To make that clearer we calculated the superconducting gap in finite temperature. Here the superconducting gap Δ in equation (3) should be replaced by $\Delta(T)$, and $\Delta(T)$ is determined by

$$\Delta(T) = V^{SC} N_F \pi T \sum_m \frac{\tilde{\Delta}}{\sqrt{\tilde{\Delta}^2 + \tilde{\omega}_m^2 + x^2}}. \quad (5)$$

where V^{SC} is the coupling constant and $\omega_m = (2m+1)\pi T$.

Solution of (2)-(5) gives the finite temperature gap $\Delta(T)$. The intra- and inter-band magnetic impurity effect to $\Delta(T)$ are shown in Fig.2. In Fig.2(a) only intra-band impurity scattering exists and $\frac{1}{\tau_1} = \frac{1}{\tau_2} \propto J_1^2$. When we increase the intra-band scattering, the finite temperature gap and the transition temperature become smaller. This case is in accordance with conventional s -wave superconductors [18]. In Fig.2(b) things will be reversed if we settle down the intra-band scattering and increase the inter-band one. $\Delta(T)$ and T_C becomes larger with J_2 increasing.

Such an effect also reflects in the transition temperature

$$\ln \frac{T_c}{T_{cp}} = \sum_{m=0} \left[\frac{1}{(m + \frac{1}{2}) \sqrt{1 - (\frac{T}{\tilde{\omega}_m})^2 + \frac{1}{\tau_S} \frac{1}{2\pi T_c}}} - \frac{1}{m + \frac{1}{2}} \right],$$

where T_c and T_{cp} are the transition temperatures with and without magnetic impurities, respectively. The numerical results of the transition temperature vs. α_0 is depicted in Fig.3. Once the $\lambda = J_2/J_1$ increasing, the depression of the transition temperature is effectively speeded up in the s -wave superconductor but slowed in the s_{\pm} -wave superconductor. In experiments, Co -doping introduces extra carriers and modifies the crystal structure [10]. As those changes may be crucial to the superconductivity, it is quite difficult to examine whether other issues may play a role in the robustness of superconductivity. However, a very recent neutron irradiation experiment on $LaO_{0.9}F_{0.1}FeAs$ provides a chance to check our theory since in this experiment both the crystal structure and carrier density of the sample are almost unchanged. The comparison is shown

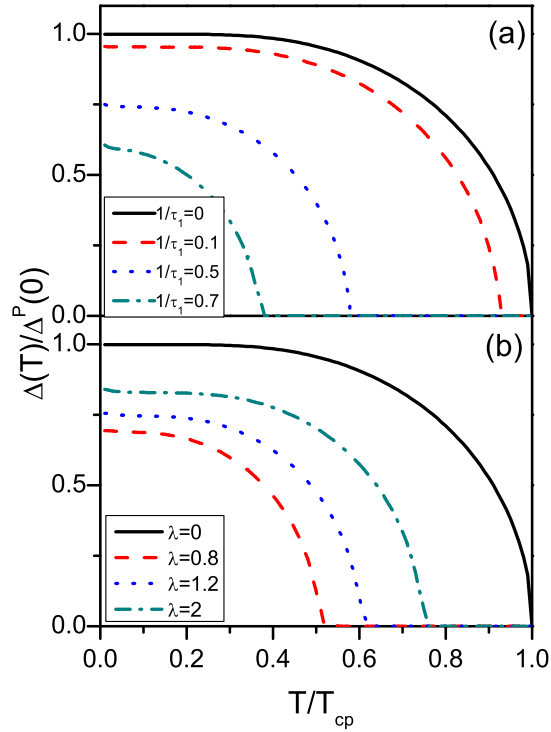


Fig. 2: (Color online) The superconducting gap in finite temperature with different intra- or inter-band impurity scattering amplitudes. The solid black line in both (a) and (b) is the two bands BCS case without impurities. $\Delta^P(0)$ is the superconducting gap without impurities in zero temperature. (a) $J_2 = 0$. (b) The solid black line: $n_{imp} = J_1 = 0$; others: $\pi n_{imp} N_F S(S+1) = 0.7$, $J_1 = 1$.

in Fig.3. The experimental data is fitted quite well with our theory quantitatively. In the real iron-based materials, with the increasing of the Co -doping, the hole pocket becomes smaller and the electron pocket becomes larger because of the shift of the chemical potential. This will weaken the inter-band magnetic scattering and preserving of T_c .

If $\lambda > 1$, T_c goes down to a finite value rather than zero when α_0 is very large. This indicates that in the Born approximation the *superconductivity can never be destroyed by magnetic impurities if the inter-band scattering is stronger than the intra-band one in the s_{\pm} -wave superconductors*. To clarify this issue further, we consider a single classical spin in an s_{\pm} -wave superconductor, which can be treated with more accuracy. The T-matrix in this case is given by

$$T = V[1 - G^0(0, \omega)V]^{-1}.$$

The energy of the bound state induced by the single magnetic impurity in an s_{\pm} superconductor is determined by

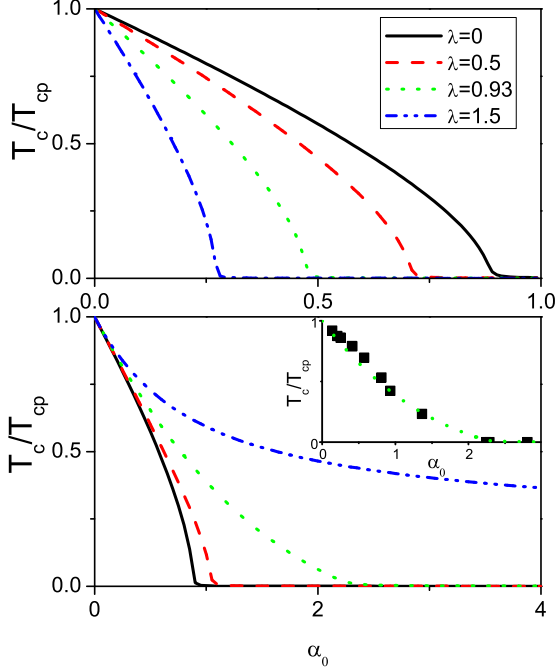


Fig. 3: (Color online) The reduced transition temperature for the conventional s -wave (above) and s_{\pm} -wave (below). When $\lambda = 0$ the conventional AG behavior is regained. Inset: fitting of the experimental data (filled squares) from Ref. [13] with $\lambda = 0.93$

the pole of the T-matrix

$$\frac{\omega_0}{\Delta} = \pm \frac{1 - \alpha_1 + \alpha_2}{\sqrt{1 + 2\alpha_1 + \alpha_1^2 - 2\alpha_1\alpha_2 + 2\alpha_2 + \alpha_2^2}}, \quad (6)$$

while the position of the bound state for the conventional s -wave superconductor is $\frac{\omega_0}{\Delta} = \pm \frac{1 - \alpha_3}{1 + \alpha_3}$ with

$$\begin{aligned} \alpha_1 &= \left(\frac{\pi J_1 S N_F}{2} \right)^2, \\ \alpha_2 &= \left(\frac{\pi J_2 S N_F}{2} \right)^2, \\ \alpha_3 &= \left[\frac{\pi (J_1 \pm J_2) S N_F}{2} \right]^2. \end{aligned}$$

If $J_2 = 0$, i.e., only the intra-band impurity scattering exists [19], the bound state energy (BSE) is $\frac{\omega_0}{\Delta} = \pm \frac{1 - \alpha_1}{1 + \alpha_1}$, which falls into the gap [20] and we recover the Yu-Shiba-Rusinov solution [21–23]. If only the inter-band impurity scattering exists, The BSE is $\frac{\omega_0}{\Delta} \rightarrow \pm 1$, i.e., locates at the gap edge. Generally, the BSE falls into the gap. Note for the conventional two-band s -wave superconductors, the bound state splits into two branches in each band due to the inter-band magnetic scattering. However, for the s_{\pm} case, there is only one bound state and increasing J_1 pushes the BSE to the Fermi energy side while increasing J_2 pushes the BSE to the gap edge side. With a finite

impurity concentration, an impurity band [22] will be expanded around the position of the BSE. The superconducting gap can be suppressed (enlarged) by increasing J_1 (J_2). This analysis supports our Born approximation result.

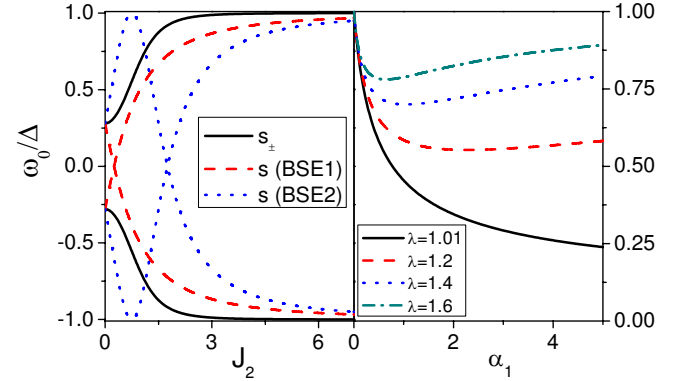


Fig. 4: (Color online) Left: The position of the bound state energy vs. the inter-band coupling constant J_2 in conventional s and s_{\pm} superconductors. The two branches of the bound states in s case are labeled as BSE1 and BSE2 and $J_1 = 0.75$. Right: Change of the position of the bound state energy with α_1 and $\lambda = J_2/J_1$

When $\lambda > 1$, from Eq.(3) we can see that

$$\begin{aligned} & \frac{1 - \alpha_1 + \alpha_2}{\sqrt{1 + 2\alpha_1 + \alpha_1^2 - 2\alpha_1\alpha_2 + 2\alpha_2 + \alpha_2^2}} \\ &= \frac{1}{\sqrt{1 + \frac{4\alpha_1}{[1 + (\lambda^2 - 1)\alpha_1]^2}}} \geq \sqrt{1 - \lambda^{-2}}, \end{aligned}$$

which means in this case the BSE has always a positive value and can never reach the Fermi level. Such fact preserves the finite superconducting gap even with a finite impurity concentration of impurities and explains why T_c goes to a finite value rather than zero with the increasing of α_0 in Fig.3. The position of the BSE with increasing α_1 and different λ is shown in the right part of Fig.4. Considering the impurity band expanded around the position of BSE [22], the region where always exists a finite gap should be in $\lambda \geq 1$. The discussion on the single impurity problem makes our conclusion to a broader region beyond the weak scattering limit.

It is well known that the magnetic impurity is a pair-breaker in the conventional spin singlet superconductors because it breaks the time-reversal symmetry and non-magnetic impurity can break the pairs in d -wave superconductors because it smears the anisotropy of the order parameter. If we neglect J_1 and look back to the effect of the inter-band impurity scattering, we find that both of the time-reversal breaking and sign reversal of the order parameters exist but canceled each other in the s_{\pm} -wave

superconductors. In fact, due to the sign reversal of the order parameters, the wave functions in different pockets have a spin up-down exchange. Therefore, the inter-band spin-flip scattering process caused by magnetic impurity is the same as the intra-band nonmagnetic scattering process which preserves the spins and does not break the pairs. This is in accordance with the "reversed AG theory" in the inter-band channel which is proposed and noticed before [24]. Though the inter-band magnetic scattering has no effect on pair breaking but J_1 can still suppress the superconducting gap and T_c . In our system which is based on one electron band and one hole band with the s_{\pm} -wave pairing symmetry, the emerge of the inter-band scattering via impurities is inevitable and makes the inter-band magnetic scattering behaves like a "pair repairer" and weakens the depression of the superconductivity.

Based on our theoretical prediction, one may distinguish the pairing symmetry in experiments by substituting magnetic ions out of but coupled to the $FeAs$ layers and the T_c depression must behave quite differently in s -wave and s_{\pm} -wave superconductors. A very recent experiment [25] showed that $BaFe_{1-x}Co_xAs_2$ is always more robust and have larger superconducting region than $BaFe_{1-x}Ni_xAs_2$, though Ni doping can result in smaller c -axis and bring more extra electrons into the superconducting layer. In another recent experiment [26], the compound $Ba_{1-x}K_xFe_2As_2$ shows a very large superconducting area with doping (from $x=0.1$ to $x=1.0$). These experiments also indicate the importance of the inter-band magnetic scattering. However, the in-plane doped magnetic impurities may affect other factors relevant to the superconductivity which make the situation unclear. One can also distinguish the s_{\pm} and conventional s pairing symmetry in two band superconductors by detecting the bound state energy. There is one bound state in s_{\pm} case but two in s case. Besides, with the increasing of J_2 , the BSE will move to the gap edge side in s_{\pm} case. In conventional s case, BSE1 will move to the Fermi edge side and quickly a quantum phase transition happens [27], but BSE2 first moves to the gap edge when $J_2 < J_1$ and then goes to the Fermi energy side when $J_2 > J_1$. Such behavior is shown in the left part of Fig.4. The position of BSE near the magnetic impurity can be detected from the tunneling spectra with a low-temperature scanning tunneling microscope (STM) which has been used to detect the Yu-Shiba-Rusinov bound state successfully [28].

In summary, the magnetic impurity effect in the two-band superconductors with a perfect nesting effect is studied for both the conventional s -wave pairing and the s_{\pm} -wave pairing. Under the condition of the same magnitude of order parameters in each band, it is found that the depression behaviors to the superconductivity with these two different pairing symmetries are quite different due to the existence of the inter-band impurity scattering, which is almost inevitable in the multi-band systems. Our theory surprisingly coincides with the neutron irradiation experiment quantitatively and we believe it can also explain why

the iron-based superconductors show high tolerance with magnetic impurities in many recent experiments. This provides an indirect method to detect the pairing symmetry of the $FeAs$ superconductors in experiments.

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